

Computer aided AFM imaging and recognition of 3D molecules

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In recent decade Atomic Force Microscopy with tip functionalized by carbon monoxide (CO) provided unique tool to experimentally image sub-molecular details of individual organic molecules [1], which is of great importance e.g. for on-surface chemistry. Most experiments are, however, up to now limited to flat aromatic molecules, due to difficulties with interpretation of highly distorted AFM images originating from non-planer molecules due to mechanical relaxation of tip or sample. These problems can be partially overcome using a simple mechanical model (Probe-Particle Model [2]) which can reproduce those distortions, therefore simulate AFM images for given molecular structure. However, this still requires laborious search for molecular structure which reproduces that particular experimental image. Instead we attempt to develop automatic tool to conduct inverse task – to recover molecular structure from given set of AFM images. Preliminary results suggest that convolutional neural network (CNN) [3] trained on simulated AFM images can learn this inverse mapping rather easily. Yet application of the method on real experimental data, and identification of atomic species remains to be a challenge.

[1] Gross, L., Mohn, F., Moll, N., Liljeroth, P., & Meyer, G., *Science* **325**(5944), 1110-1114 (2009).

[2] Hapala, P., Kichin, G., Wagner, C., Tautz, F. S., Temirov, R., & Jelinek, *Physical Review B* **90**(8), 085421 (2014).

[3] Lecun, Y., Bottou, L., Bengio, Y., & Haffner, P., *Proceedings of the IEEE* **86**(11), 2278-2324 (1998).